

MICROWAVE AND MILLIMETER WAVE SPECTRUM OF FIVE CONFORMERS OF CYSTEAMINE AND SEARCH IN SAGITTARIUS B2(N)

WENTAO SONG, ASSIMO MARIS, LUCA EVANGELISTI, DINGDING LV, SONIA MELANDRI, *Dipartimento di Chimica G. Ciamician, Università di Bologna, Bologna, Italy.*

Cysteamine ($\text{NH}_2\text{CH}_2\text{CH}_2\text{SH}$), is the precursor of cysteine (a sulfur-containing amino acid) in cell metabolism. As such it is interesting from the chemical and biochemical point of view and as a target interstellar molecule which could be a precursor of amino acid formation. Its rotational spectrum has already been investigated in the 18-40 GHz frequency region and two conformers and their vibrational satellites were characterized, but the sparse frequency coverage prevents their accurate predictions in higher frequency ranges. Moreover, conformational potential energy scans performed at the B3LYP-GD3(BJ)/def2-TZVP level of calculation suggest the existence of more stable conformers. To fill the lack of its spectroscopic knowledge, we have investigated the pure rotational spectrum of cysteamine by means of a Pulsed Jet Fourier transform microwave spectrometer and a Stark modulated free-jet millimeter-wave absorption spectrometer with frequency ranges of 6.5-18 GHz (46.12-16.66 mm) and 59.6-110.0 GHz (5.03-2.72 mm), respectively. According to theoretical predictions, five conformers, belonging to the *gauche* skeletal arrangement ($\angle\text{NCCS} \approx 60^\circ$) have been observed, and for three of them also the ^{34}S isotopologues were observed in natural abundance. Some of the detected lines shown a hyperfine structure ($\Delta\nu \leq 1$ MHz) due to the nuclear quadrupole interaction of the ^{14}N atom. Altogether, 336 transition lines of the five parent species and 63 lines of the three ^{34}S isotopologues conformers were assigned to fit the rotational constants, quartic centrifugal distortion constants and the ^{14}N nuclear quadrupole coupling constants. New laboratory data of cysteamine provided very precise values of the spectroscopic constants that can be used to search for cysteamine in astronomical surveys. As a first try, we have looked towards the north core of the giant molecular cloud Sagittarius B2 (N) (Sgr B2(N)), in the band 3 (3.6-2.6 mm), exploiting Belloche's data stored in the public available Atacama Large Millimeter/submillimeter Array (ALMA) archive (project 2016.1.00074.S).